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Generalization of the Edgeworth and Gram-Charlier series and quasi-probability densities

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Abstract. The main historical purpose of the standard Gram-Charlier and Edgeworth series is to “correct” a Gaussian distributions when new information, such as moments, is given which does not match those of the Gaussian. These methods relate a probability distribution to a Gaussian by way of an operator transformation that is a function of the differentiation operator. We use the methods of the phase-space formulation of quantum mechanics to generalize these methods. We generalize in two ways. First, we relate any two probability distributions by way differentiation operator. Second, we generalize to the case where the differentiation operator is replaced by an arbitrary Hermitian operator. The generalization results in a unified approach for the operator transformation of probability densities. Also, when the Edgeworth and Gram-Charlier series are truncated, the resulting approximation is generally not manifestly positive. We present methods where the truncated series remain manifestly positive.

1 Introduction

Quantum phase space distributions such as the Wigner distribution and its generalizations have been used in many fields of physics and engineering. Standard quantum mechanics can be formulated in terms of these position momentum distributions, and the resulting formulation is called the phase-space formulation of quantum mechanics [13, 5]. A similar formulation is used to describe time varying spectra and that field is called time-frequency analysis [4].

The distributions involved are often called quasi-distributions because they do not satisfy all the properties of a probability density. In particular, they may go negative. Many of the results of the phase-space formulation and time-frequency analysis seem peculiar and are unlike methods that have been developed in standard probability theory. However, in standard probability theory there are the Edgeworth and Gram-Charlier series, which are methods for correcting probability distributions [18]. These methods are similar to the methods used in quasi-probability distribution theory. We therefore argue that the operator methods used in quantum mechanics, and in particular in the phase-space formulation of quantum mechanics, are fruitful in generalizing the standard Edgeworth/Gram-Charlier series.

2 Notation and mathematical preliminaries

Operators will be denoted by script letters as, for example,

$$\mathcal{D} = \frac{1}{i} \frac{d}{dx} \quad (1)$$

However, because of convention, the differentiation operator will be denoted by D

$$D = \frac{d}{dx} = i\mathcal{D} \quad (2)$$

If an operator is operating on function of variables other than x , then we denote that by a subscript. For example

$$D_y = \frac{d}{dy} \quad (3)$$

All integrals go from $-\infty$ to ∞ unless others noted

$$\int = \int_{-\infty}^{\infty} \quad (4)$$

Hermitian operators. A operator, \mathcal{A} , is Hermitian if for any two functions g and f , we have

$$\int g^*(x) \mathcal{A}f(x) dx = \int f(x) \{\mathcal{A}g(x)\}^* dx \quad (5)$$

The phrase Hermitian operator is used in physics, but in other fields the term symmetric operator is often used. In addition, the term “self adjoint operator” is used.

Functions of operators. There are many ways to define functions of operators. We mention two of them. A function of an operator, $f(\mathcal{A})$, is defined by first expanding the ordinary function $f(x)$ in a power series

$$f(x) = \sum_{n=0}^{\infty} f_n x^n \quad (6)$$

and then defining $f(\mathcal{A})$ by substituting \mathcal{A} for x ,

$$f(\mathcal{A}) = \sum_{n=0}^{\infty} f_n \mathcal{A}^n \quad (7)$$

A second way is by the Fourier transform, $\hat{f}(k)$, of $f(x)$,

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int f(x) e^{-ixk} dx \quad (8)$$

with

$$f(x) = \frac{1}{\sqrt{2\pi}} \int \hat{f}(k) e^{ixk} dk \quad (9)$$

One then defines $f(\mathcal{A})$ by substituting \mathcal{A} for x in Eq. (9)

$$f(\mathcal{A}) = \frac{1}{\sqrt{2\pi}} \int \hat{f}(k) e^{ik\mathcal{A}} dk \quad (10)$$

Expansion of functions and transforms. For a Hermitian operator, \mathcal{A} , the eigenvalue problem

$$\mathcal{A} u_{\theta}(x) = \theta u_{\theta}(x) \quad (11)$$

produces real eigenvalues, θ , and eigenfunctions, $u_{\theta}(x)$, that are complete and orthogonal

$$\int u_{\theta'}^*(x) u_{\theta}(x) dx = \delta(\theta - \theta') \quad (12)$$

$$\int u_{\theta}^*(x') u_{\theta}(x) d\theta = \delta(x - x') \quad (13)$$

Any function, $f(x)$, can be expanded as

$$f(x) = \int F(\theta) u_{\theta}(x) d\theta \quad (14)$$

where

$$F(\theta) = \int f(x) u_{\theta}^*(x) dx \quad (15)$$

The function $F(\theta)$ is called the transform of $f(x)$ in the θ representation

Function of an operator operating on an eigenfunction and on an arbitrary function. If $u_\theta(x)$ are the eigenfunctions of the operator \mathcal{A} , then for a function of this operator, $f(\mathcal{A})$, we have that

$$f(\mathcal{A})u_\theta(x) = f(\theta)u_\theta(x) \quad (16)$$

This follows straightforwardly by expanding $f(\mathcal{A})$ in a Taylor series and using Eq. (11) repeatedly.

For example suppose $u_\theta(x) = e^{-ix\theta}$ are the eigenfunctions of the operator iD ,

$$iDe^{-ix\theta} = \theta e^{-ix\theta} \quad (17)$$

then we have that for any function $\Omega(\theta)$

$$\Omega(iD)e^{-ix\theta} = \Omega(\theta)e^{-ix\theta} \quad (18)$$

Eq. (16) allows one to evaluate the operation of $f(\mathcal{A})$ on an arbitrary function, $g(x)$. First, expand $g(x)$ as

$$g(x) = \int G(\theta)u_\theta(x) d\theta \quad (19)$$

where the transform, $G(\theta)$, is given by

$$G(\theta) = \int g(x)u_\theta^*(x) dx \quad (20)$$

Now, consider

$$f(\mathcal{A})g(x) = f(\mathcal{A}) \int G(\theta)u_\theta(x) d\theta \quad (21)$$

$$= \int G(\theta)f(\mathcal{A})u_\theta(x) d\theta \quad (22)$$

Using Eq. (16) we then have that

$$f(\mathcal{A})g(x) = \int G(\theta)f(\theta)u_\theta(x) d\theta \quad (23)$$

If we further substitute for $G(\theta)$ as given by Eq. (20), then

$$f(\mathcal{A})g(x) = \iint g(x')u_\theta^*(x')f(\theta)u_\theta(x) d\theta dx' \quad (24)$$

which can be written as

$$f(\mathcal{A})g(x) = \int g(x')r(x', x)dx' \quad (25)$$

where

$$r(x', x) = \int u_\theta^*(x')f(\theta)u_\theta(x) d\theta \quad (26)$$

Translation operator. The operator that translates a function is $e^{\theta D}$,

$$e^{\theta D}f(x) = f(x + \theta) \quad (27)$$

The operator $e^{-aD+bD^2/2}$. The action of the operator on an arbitrary function is

$$e^{-aD+bD^2/2}f(x) = \frac{1}{\sqrt{2\pi b}} \int e^{-\frac{(x'-x+a)^2}{2b}} f(x') dx' \quad (28)$$

Hermite polynomials and functions. In physics and engineering the standard definition for the Hermite polynomials, $H_n(x)$, is [2, 16]

$$H_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k n!}{k!(n-2k)!} (2x)^{n-2k} = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad (29)$$

and the Hermite functions are defined by

$$u_n(x) = \frac{1}{\sqrt{2^n n! \pi^{1/4}}} H_n(x) e^{-x^2/2} \quad (30)$$

The Hermite functions are orthonormal and complete,

$$\int u_n(x)u_k(x) dx = \delta_{nk} \quad (31)$$

$$\sum_{n=0}^{\infty} u_n(x)u_n(x') = \delta(x' - x) \quad (32)$$

In the probability literature, the Hermite polynomials with notation $He_n(x)$, are defined slightly differently [18],

$$He_n(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2} \quad (33)$$

The relation between the two definitions is

$$H_n(x) = 2^{n/2} He_n(\sqrt{2}x) \quad (34)$$

$$He_n(x) = 2^{-n/2} H_n(x/\sqrt{2}) \quad (35)$$

It is also useful to define the functions

$$u_n(x; m, \alpha) = \sqrt{\frac{\alpha}{2^n n! \sqrt{\pi}}} H_n(\alpha(x - m)) e^{-\alpha^2(x - m)^2/2} \quad (36)$$

where m and α are real numbers and where $H_n(\alpha(x - m))$ are translated and scaled Hermite polynomials given by

$$H_n(\alpha(x - m)) = \frac{(-1)^n}{\alpha^n} e^{\alpha^2(x - m)^2} \frac{d^n}{dx^n} e^{-\alpha^2(x - m)^2} \quad (37)$$

These functions are also orthonormal

$$\int u_n(x; m, \alpha) u_k(x; m, \alpha) dx = \delta_{nk} \quad (38)$$

Characteristic function, moment, cumulants. As standard, the characteristic function, $M(\theta)$, of a probability distribution $P(x)$ is defined by [15]

$$M(\theta) = \int e^{i\theta x} P(x) dx \quad (39)$$

The probability distribution may be obtained from the characteristic function by way of

$$P(x) = \frac{1}{2\pi} \int e^{-i\theta x} M(\theta) d\theta \quad (40)$$

By expanding the exponential in Eq. (39) one has

$$M(\theta) = \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \langle x^n \rangle \quad (41)$$

where $\langle x^n \rangle$ are the moments of $P(x)$.

The cumulant form of the characteristic functions is where one expands the log of the characteristic function

$$\ln M(\theta) = \sum_{n=1}^{\infty} \kappa_n \frac{i^n}{n!} \theta^n \quad (42)$$

where κ_n are called the cumulants. Therefore

$$M(\theta) = \exp \left[\sum_{n=1}^{\infty} \kappa_n \frac{i^n}{n!} \theta^n \right] = \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \langle x^n \rangle \quad (43)$$

The relation between the moments and cumulants is well known [18].

3 Quasi distributions¹

Suppose we have an ordinary function of two variables $g(x, k)$ and a corresponding operator $\mathbf{G}(\mathcal{X}, \mathcal{K})$ where the operators \mathcal{X} and \mathcal{K} are

$$\mathcal{X} = \begin{cases} x & \text{in the } x \text{ representation} \\ i \frac{d}{dk} & \text{in the Fourier representation} \end{cases} \quad (44)$$

$$\mathcal{K} = \begin{cases} \frac{1}{i} \frac{d}{dx} & \text{in the } x \text{ representation} \\ k & \text{in the Fourier representation} \end{cases} \quad (45)$$

The fundamental relation between \mathcal{X} and \mathcal{K} is the commutation relation,

$$[\mathcal{X}, \mathcal{K}] = \mathcal{X}\mathcal{K} - \mathcal{K}\mathcal{X} = i \quad (46)$$

The relation between the ordinary function and the operator is symbolized by

$$g(x, k) \leftrightarrow \mathbf{G}(\mathcal{X}, \mathcal{K}) \quad (47)$$

The relation between $g(x, k)$ and $\mathbf{G}(\mathcal{X}, \mathcal{K})$ is called a correspondence rule.

In quantum mechanics, we calculate expectation value by way of [1, 16]

$$\langle \mathbf{G}(\mathcal{X}, \mathcal{K}) \rangle = \int \psi^*(x) \mathbf{G}(\mathcal{X}, \mathcal{K}) \psi(x) dx \quad (48)$$

where $\psi(x)$ is the state function of the system. Classically, if we have a joint density of x and k , say $C(x, k)$, the expectation value of $g(x, k)$ is calculated by phase space integrations

$$\langle g(x, k) \rangle = \iint g(x, k) C(x, k) dx dk \quad (49)$$

We want the two approaches to give the same answer,

$$\langle \mathbf{G}(\mathcal{X}, \mathcal{K}) \rangle = \langle g(x, k) \rangle \quad (50)$$

There are an infinite number of quasi-distributions, and all bilinear ones may be obtained from [3, 13, 4, 5]

$$C(x, k) = \frac{1}{4\pi^2} \iiint \psi^*(u - \frac{1}{2}\tau) \psi(u + \frac{1}{2}\tau) \Phi(\theta, \tau) e^{-i\theta x - i\tau k + i\theta u} du d\tau d\theta \quad (51)$$

¹This section may be skipped for those readers who are not interested in the quantum mechanics motivation of the subsequent sections.

where $\Phi(\theta, \tau)$ is the kernel function that characterizes the distribution. Eq. (51) may be expressed in terms of a characteristic function $M(\theta, \tau)$,

$$M(\theta, \tau) = \iint e^{i\theta x + i\tau k} C(x, k) dx dk \quad (52)$$

The distribution function is then given by

$$C(x, k) = \frac{1}{4\pi^2} \iint M(\theta, \tau) e^{-i\theta x - i\tau k} d\theta d\tau \quad (53)$$

Substituting Eq. (51) into Eq. (52) one has

$$M(\theta, \tau) = \Phi(\theta, \tau) \int \psi^*(x - \frac{1}{2}\tau) e^{i\theta x} \psi(x + \frac{1}{2}\tau) dx \quad (54)$$

The general correspondence rule is

$$\mathbf{G}(\mathcal{X}, \mathcal{K}) = \iint \widehat{g}(\theta, \tau) \Phi(\theta, \tau) e^{i\theta \mathcal{X} + i\tau \mathcal{K}} d\theta d\tau \quad (55)$$

where

$$\widehat{g}(\theta, \tau) = \frac{1}{4\pi^2} \iint g(x, k) e^{-i\theta x - i\tau k} dx dk \quad (56)$$

It then follows that the quantum expectation value calculated gives the same answer as the classical one, that is

$$\iint g(x, k) C(x, k) dx dk = \int \psi^*(x) \mathbf{G}(\mathcal{X}, \mathcal{K}) \psi(x) dx \quad (57)$$

We also want

$$\int W(x, k) dk = |\psi(x)|^2 \quad (58)$$

$$\int W(x, k) dx = |\varphi(k)|^2 \quad (59)$$

where $|\psi(x)|^2$ is the probability distribution of position and $|\varphi(k)|^2$ is the probability distribution of momentum, where the momentum wave function is

$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x) e^{-ixk} dx \quad (60)$$

The first quantum phase space quasi-distribution proposed was that of Wigner [22]

$$W(x, k) = \frac{1}{2\pi} \int \psi^*(x - \frac{1}{2}\tau) \psi(x + \frac{1}{2}\tau) e^{-i\tau k} d\tau \quad (61)$$

If we take $\Phi(\theta, \tau) = 1$ in Eq. (51) we obtain the Wigner distribution. Moyal [17] showed that if we use the Wigner distribution, Eq.(57) will hold if we associate the classical function with the Weyl operator [20, 5, 23], which is defined by

$$\mathbf{G}_W(\mathcal{X}, \mathcal{K}) = \iint \hat{g}(\theta, \tau) e^{i\theta\mathcal{X} + i\tau\mathcal{K}} d\theta d\tau \quad (62)$$

Transformation properties of quasi-distributions. The important result for our subsequent considerations is the relation and transformation properties between distributions. If we have two distributions $C_1(x, k)$ and $C_2(x, k)$ characterized by the kernels Φ_1 and Φ_2 , then the relation between them is [3, 7, 13]

$$C_2(x, k) = \iint g_{21}(x' - x, k' - k) C_1(x', k') dx' dk' \quad (63)$$

with

$$g_{21}(x, k) = \frac{1}{4\pi^2} \iint \frac{\Phi_2(\theta, \tau)}{\Phi_1(\theta, \tau)} e^{i\theta x + i\tau k} d\theta d\tau \quad (64)$$

Equivalently one can show that,

$$C_2(x, k) = \frac{\Phi_2(i\frac{\partial}{\partial x}, i\frac{\partial}{\partial k})}{\Phi_1(i\frac{\partial}{\partial x}, i\frac{\partial}{\partial k})} C_1(x, k) \quad (65)$$

This equation relates two distributions by an operator transformation.

3.1 Edgeworth series

The main historical purpose of the Gram-Charlier and Edgeworth series is to “correct” a Gaussian distributions when new information, such as moments, are given where the new moments do not match the moment of the Gaussian. One form of the standard Edgeworth series is

$$P_2(x) = \exp \left[-(\kappa_1^{(2)} - m)D + \frac{1}{2}(\kappa_2^{(2)} - \sigma^2)D^2 + \sum_{n=3}^{\infty} \kappa_n^{(2)} \frac{(-i)^n}{n!} D^n \right] N(m, \sigma^2) \quad (66)$$

where $N(m, \sigma^2)$ is the normal distribution

$$N(m, \sigma^2) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp \left[-\frac{(x - m)^2}{2\sigma^2} \right] \quad (67)$$

and $\kappa_n^{(2)}$ are the cumulates of the probability distribution $P_2(x)$.

Although we have given the Edgeworth series for the one dimensional case, a similar relation holds for the two dimensional case. Now, notice that in Eq. (66) the probability distributions $P_2(x)$ and $N(m, \sigma^2)$ are related by an operator transformation, and that is exactly how the two distributions in Eq. (65) are related.

The issues we address in this paper are, can one generalize Eq. (66) so that the starting distribution is arbitrary rather than Gaussian? Second, can the operator D be replaced by other operators?

4 Generalization one: The relation between distributions involving D

We show that any two probability densities $P_1(x)$ and $P_2(x)$ may be related by [8, 9]

$$P_2(x) = \Omega(iD)P_1(x) \quad (68)$$

where $\Omega(iD)$ is function of the operator iD that is given explicitly below. Suppose $M_1(x)$ and $M_2(x)$ are the corresponding characteristic functions to the two densities,

$$M_1(\theta) = \int e^{i\theta x} P_1(x) dx \quad ; \quad P_1(x) = \frac{1}{2\pi} \int e^{-i\theta x} M_1(\theta) d\theta \quad (69)$$

$$M_2(\theta) = \int e^{i\theta x} P_2(x) dx \quad ; \quad P_2(x) = \frac{1}{2\pi} \int e^{-i\theta x} M_2(\theta) d\theta \quad (70)$$

We write

$$M_2(\theta) = \frac{M_2(\theta)}{M_1(\theta)} M_1(\theta) = \Omega(\theta) M_1(\theta) \quad (71)$$

where

$$\Omega(\theta) = \frac{M_2(\theta)}{M_1(\theta)} \quad (72)$$

The probability distribution, $P_2(x)$, is then

$$P_2(x) = \frac{1}{2\pi} \int e^{-ix\theta} M_2(\theta) d\theta \quad (73)$$

$$= \frac{1}{2\pi} \int e^{-ix\theta} \frac{M_2(\theta)}{M_1(\theta)} M_1(\theta) d\theta \quad (74)$$

$$= \frac{1}{2\pi} \int e^{-ix\theta} \Omega(\theta) M_1(\theta) d\theta \quad (75)$$

Using Eq. (18) we have

$$\Omega(\theta)e^{-ix\theta} = \Omega(iD)e^{-ix\theta} \quad (76)$$

and therefore

$$P_2(x) = \frac{1}{2\pi} \int \Omega(iD)e^{-ix\theta} M_1(\theta) d\theta \quad (77)$$

$$= \Omega(iD) \frac{1}{2\pi} \int e^{-ix\theta} M_1(\theta) d\theta \quad (78)$$

$$= \Omega(iD) P_1(x) \quad (79)$$

which is Eq. (68).

Two Dimensions. For the two dimensional case, the characteristic function, $M(\theta, \tau)$, and density, $P(x, y)$, are related by

$$M(\theta, \tau) = \iint e^{i\theta x + i\tau y} P(x, y) dx dy \quad (80)$$

$$P(x, y) = \frac{1}{4\pi^2} \iint M(\theta, \tau) e^{-i\theta x - i\tau y} d\theta d\tau \quad (81)$$

Suppose we have two, two dimensional densities, $P_1(x, y)$ and $P_2(x, y)$ with corresponding characteristic functions $M_1(\theta, \tau)$ and $M_2(\theta, \tau)$, we set

$$\Omega(\theta, \tau) = \frac{M_2(\theta, \tau)}{M_1(\theta, \tau)} \quad (82)$$

The same proof used for the one dimensional case leads to

$$P_2(x, y) = \Omega(D_x, D_y) P_1(x, y) \quad (83)$$

Generalization to higher dimensions is straightforward.

4.1 Generalized Edgeworth type series

We now obtain a generalized Edgeworth series. For two densities $P_1(x)$ and $P_2(x)$ we write the corresponding characteristic functions in cumulant form,

$$M_1(\theta) = \exp \left[\sum_{n=1}^{\infty} \kappa_n^{(1)} \frac{i^n}{n!} \theta^n \right] \quad (84)$$

$$M_2(\theta) = \exp \left[\sum_{n=1}^{\infty} \kappa_n^{(2)} \frac{i^n}{n!} \theta^n \right] \quad (85)$$

where $\kappa_n^{(1)}$ and $\kappa_n^{(2)}$ are the respective cumulates of $P_1(x)$ and $P_2(x)$. Using Eq. (72) we have

$$\Omega(\theta) = \frac{M_2(\theta)}{M_1(\theta)} = \frac{\exp \left[\sum_{n=1}^{\infty} \kappa_n^{(2)} \frac{i^n}{n!} \theta^n \right]}{\exp \left[\sum_{n=1}^{\infty} \kappa_n^{(1)} \frac{i^n}{n!} \theta^n \right]} \quad (86)$$

or

$$\Omega(\theta) = \exp \left[\sum_{n=1}^{\infty} (\kappa_n^{(2)} - \kappa_n^{(1)}) \frac{i^n}{n!} \theta^n \right] \quad (87)$$

Eq. (68) then gives

$$P_2(x) = \exp \left[\sum_{n=1}^{\infty} (\kappa_n^{(2)} - \kappa_n^{(1)}) \frac{i^n}{n!} (iD)^n \right] P_1(x) \quad (88)$$

or

$$P_2(x) = \exp \left[\sum_{n=1}^{\infty} (\kappa_n^{(2)} - \kappa_n^{(1)}) \frac{(-1)^n}{n!} D^n \right] P_1(x) \quad (89)$$

We call Eq. (89) the generalized Edgeworth series since it relates any two probability densities.

5 Approximation

We now discuss two approximations.

5.1 First approximation

We expand the operator in Eq. (89) in a power series

$$\begin{aligned} \exp \left[\sum_{n=1}^{\infty} (\kappa_n^{(2)} - \kappa_n^{(1)}) \frac{(-1)^n}{n!} D^n \right] &= 1 - a_1 D + \frac{1}{2} a_2 D^2 - \frac{1}{6} a_3 D^3 \\ &+ \frac{1}{24} a_4 D^4 - \frac{1}{120} a_5 D^5 + \frac{1}{720} a_6 D^6 + \dots \end{aligned} \quad (90)$$

where we have kept terms up to D^6 . Therefore the approximation is

$$P_2(x) \sim \left[1 - a_1 D + \frac{1}{2} a_2 D^2 - \frac{1}{6} a_3 D^3 + \frac{1}{24} a_4 D^4 - \frac{1}{120} a_5 D^5 + \frac{1}{720} a_6 D^6 \dots \right] P_1(x) \quad (91)$$

For notational convenience we define

$$\eta_n = \kappa_n^{(2)} - \kappa_n^{(1)} \quad (92)$$

One can take advantage of the relation between cumulates and moments [18] to write that

$$a_1 = \eta_1 \quad (93)$$

$$a_2 = \eta_2 + \eta_1^2 \quad (94)$$

$$a_3 = \eta_3 + 3\eta_2\eta_1 + \eta_1^3 \quad (95)$$

$$a_4 = \eta_4 + 4\eta_3\eta_1 + 3\eta_2^2 + 6\eta_2\eta_1^2 + \eta_1^4 \quad (96)$$

$$a_5 = \eta_5 + 5\eta_4\eta_1 + 10\eta_3\eta_2 + 10\eta_3\eta_1^2 + 15\eta_2^2\eta_1 + 10\eta_2\eta_1^3 + \eta_1^5 \quad (97)$$

$$a_6 = \eta_6 + 6\eta_5\eta_1 + 15\eta_4\eta_2 + 15\eta_4\eta_1^2 + 10\eta_3^2 \quad (98)$$

$$+ 60\eta_3\eta_2\eta_1 + 20\eta_3\eta_1^3 + 15\eta_2^3 + 45\eta_2^2\eta_1^2 + 15\eta_2\eta_1^4 + \eta_1^6 \quad (99)$$

If we assume that $P_1(x)$ is standardized, that is,

$$\kappa_1^{(1)} = 0 \quad \kappa_2^{(1)} = 1 \quad (100)$$

then

$$a_1 = \kappa_1^{(2)} \quad (101)$$

$$a_2 = \left(\kappa_2^{(2)} - 1\right) + \left(\kappa_1^{(2)}\right)^2 \quad (102)$$

$$a_3 = \eta_3 + 3\left(\kappa_2^{(2)} - 1\right)\kappa_1^{(2)} + \left(\kappa_1^{(2)}\right)^3 \quad (103)$$

$$a_4 = \eta_4 + 4\eta_3\kappa_1^{(2)} + 3\left(\kappa_2^{(2)} - 1\right)^2 + 6\left(\kappa_2^{(2)} - 1\right) + \left(\kappa_1^{(2)}\right)^4 \quad (104)$$

$$a_5 = \eta_5 + 5\eta_4\kappa_1^{(2)} + 10\eta_3\left(\kappa_2^{(2)} - 1\right) + 10\eta_3\left(\kappa_1^{(2)}\right)^2 + 15\left(\kappa_2^{(2)} - 1\right)^2\kappa_1^{(2)} \quad (105)$$

$$+ 10\left(\kappa_2^{(2)} - 1\right)\left(\kappa_1^{(2)}\right)^3 + \left(\kappa_1^{(2)}\right)^5 \quad (106)$$

$$a_6 = \eta_6 + 6\eta_5\kappa_1^{(2)} + 15\eta_4\left(\kappa_2^{(2)} - 1\right) + 15\eta_4\left(\kappa_1^{(2)}\right)^2 + 10\eta_3^2 + 60\eta_3\left(\kappa_2^{(2)} - 1\right)\kappa_1^{(2)} \quad (107)$$

$$+ 20\eta_3\left(\kappa_1^{(2)}\right)^3 + 15\left(\kappa_2^{(2)} - 1\right)^3 + 45\left(\kappa_2^{(2)} - 1\right)^2\left(\kappa_1^{(2)}\right)^2 + 15\left(\kappa_2^{(2)} - 1\right)\left(\kappa_1^{(2)}\right)^4 + \left(\kappa_1^{(2)}\right)^6 \quad (108)$$

If we further assume that $P_2(x)$ is also standardized

$$\kappa_1^{(2)} = 0 \quad \kappa_2^{(2)} = 1 \quad (109)$$

then

$$a_1 = 0 \quad (110)$$

$$a_2 = 0 \quad (111)$$

$$a_3 = \eta_3 \quad (112)$$

$$a_4 = \eta_4 \quad (113)$$

$$a_5 = \eta_5 \quad (114)$$

$$a_6 = \eta_6 + 10\eta_3^2 \quad (115)$$

Explicitly,

$$P_2(x) \sim \left[1 - \frac{\eta_3}{6} D^3 + \frac{\eta_4}{24} D^4 - \frac{\eta_5}{120} D^5 + \frac{\eta_6 + 10\eta_3^2}{720} D^6 + \dots \right] P_1(x) \quad (116)$$

This the same form as the standard expansion except that in the standard case $P_1(x)$ is Gaussian [18].

5.2 Second approximation

Consider writing Eq. (89) in the following form

$$P_2(x) = \exp \left[\sum_{n=1}^{\infty} \eta_n \frac{(-1)^n}{n!} D^n \right] P_1(x) \quad (117)$$

$$= \exp \left[-\eta_1 D + \frac{1}{2} \eta_2 D^2 \right] \exp \left[\sum_{n=3}^{\infty} \eta_n \frac{(-1)^n}{n!} D^n \right] P_1(x) \quad (118)$$

Using Eq. (28) we have,

$$\begin{aligned} & \exp \left[-\eta_1 D + \frac{1}{2} \eta_2 D^2 \right] f(x) \\ &= \frac{1}{\sqrt{2\pi\eta_2}} \int \exp \left[-\frac{(x' - x + \eta_1)^2}{2\eta_2} \right] f(x') dx' \end{aligned} \quad (119)$$

and therefore

$$P_2(x) = \frac{1}{\sqrt{2\pi\eta_2}} \int \exp \left[-\frac{(x' - x + \eta_1)^2}{2\eta_2} \right] \exp \left[\sum_{n=3}^{\infty} \eta_n \frac{(-1)^n}{n!} D_{x'}^n \right] P_1(x') dx' \quad (120)$$

This is still exact. If we now expand up to 6th order in D ,

$$\exp \left[\sum_{n=3}^{\infty} \eta_n \frac{(-1)^n}{n!} D_{x'}^n \right] \sim \left[1 - \frac{\eta_3}{6} D_{x'}^3 + \frac{\eta_4}{24} D_{x'}^4 - \frac{\eta_5}{120} D_{x'}^5 + \frac{\eta_6 + 10\eta_3^2}{720} D_{x'}^6 \dots \right] \quad (121)$$

we obtain

$$P_2(x) = \frac{1}{\sqrt{2\pi\eta_2}} \int \exp \left[-\frac{(x' - x + \eta_1)^2}{2\eta_2} \right] \left[1 - \frac{\eta_3}{6} D_{x'}^3 + \frac{\eta_4}{24} D_{x'}^4 - \frac{\eta_5}{120} D_{x'}^5 + \frac{\eta_6 + 10\eta_3^2}{720} D_{x'}^6 \dots \right] P_1(x') dx' \quad (122)$$

5.3 Gaussian case

If we take $P_1(x)$ to be Gaussian,

$$P_1(x) = N(m, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(x - m)^2}{2\sigma^2} \right] \quad (123)$$

then Eq. (89) gives

$$P_2(x) = \exp \left[\sum_{n=1}^{\infty} (\kappa_n^{(2)} - \kappa_n^{(1)}) \frac{(-1)^n}{n!} D^n \right] N(m, \sigma^2) \quad (124)$$

But for a Gaussian, there are only two nonzero cumulants, $\kappa_1 = m$, $\kappa_2 = \sigma^2$, and therefore

$$P_2(x) = \exp \left[-(\kappa_1^{(2)} - m)D + \frac{1}{2}(\kappa_2^{(2)} - \sigma^2)D^2 + \sum_{n=3}^{\infty} \kappa_n^{(2)} \frac{(-i)^n}{n!} D^n \right] N(m, \sigma^2) \quad (125)$$

which is the standard Edgeworth series [18].

If we consider the standardized Gaussian, where $m = 0$ and $\sigma = 1$, then

$$P_2(x) = \exp \left[-\kappa_1^{(2)} D + \frac{1}{2}(\kappa_2^{(2)} - 1)D^2 + \sum_{n=3}^{\infty} \kappa_n^{(2)} \frac{(-i)^n}{n!} D^n \right] N(0, 1) \quad (126)$$

Furthermore, if we want $P_2(x)$ to be standardized, that is, to have zero mean and unit standard deviation,

$$\kappa_1^{(2)} = 0 \quad \kappa_2^{(2)} = 1 \quad (127)$$

then

$$P_2(x) = \exp \left[\sum_{n=3}^{\infty} \kappa_n^{(2)} \frac{(-i)^n}{n!} D^n \right] N(0, 1) \quad (128)$$

and

$$P_2(x) \sim \left[1 - \frac{1}{6}\kappa_3^{(2)}D^3 + \frac{1}{24}\kappa_4^{(2)}D^4 - \frac{1}{120}\kappa_5^{(2)}D^5 + \frac{\kappa_6^{(2)} + 10\left(\kappa_3^{(2)}\right)^2}{720}D^6 \dots \right] N(0, 1) \quad (129)$$

Since

$$D^n e^{-x^2/2} = (-1)^n e^{-x^2/2} He_n(x) \quad (130)$$

we have

$$\begin{aligned} P_2(x) \sim & \left[1 + \frac{1}{6}\kappa_3^{(2)}He_3(x) + \frac{1}{24}\kappa_4^{(2)}He_4(x) + \frac{1}{120}\kappa_5^{(2)}He_5(x) \right. \\ & \left. + \frac{1}{720}\left(\kappa_6^{(2)} + 10\left(\kappa_3^{(2)}\right)^2\right)He_6(x) + \dots \right] N(0, 1) \end{aligned} \quad (131)$$

which is a well known result [18].

5.4 Generalized Gram-Charlier

We expand $\Omega(\theta)$ as given by Eq. (72) in terms of some complete set of functions, say $v_n(x)$

$$\Omega(\theta) = \frac{M_2(\theta)}{M_1(\theta)} = \sum_{n=0}^{\infty} q_n v_n(\theta) \quad (132)$$

If $v_n(\theta)$ are orthonormal, then

$$q_n = \int \frac{M_2(\theta)}{M_1(\theta)} v_n^*(\theta) d\theta \quad (133)$$

However that does not have to be the case, for example, we can expand $\Omega(\theta)$ in a power series

$$\Omega(\theta) = \frac{M_2(\theta)}{M_1(\theta)} = \sum_{n=0}^{\infty} a_n \theta^n \quad (134)$$

in which case

$$a_n = \frac{1}{n!} D^n \frac{M_2(\theta)}{M_1(\theta)} \Big|_{\theta=0} \quad (135)$$

Using Eq. (132) we have, for Eq. (68)

$$P_2(x) = \sum_{n=0}^{\infty} q_n v_n(iD) P_1(x) \quad (136)$$

We call this the generalized Gram-Charlier. For the specific case of a power series we have

$$P_2(x) = \sum_{n=0}^{\infty} a_n i^n D^n P_1(x) \quad (137)$$

5.4.1 Gaussian case

To obtain the standard Gram Charlier we take P_1 to be the the normal distribution

$$P_1 = N(m, \sigma^2) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp \left[-\frac{(x-m)^2}{2\sigma^2} \right] \quad (138)$$

Using Eq. (132) we then have

$$P_2(x) = \sum_{n=0}^{\infty} a_n i^n D^n N(m, \sigma^2) \quad (139)$$

Using the fact that

$$i^n D^n N(m, \sigma^2) = (-i\alpha)^n H_n(\alpha(x-m)) N(m, \sigma^2) \quad (140)$$

where for convenience we have set

$$\alpha = \sqrt{\frac{1}{2\sigma^2}} \quad \sigma^2 = \frac{1}{2\alpha^2} \quad (141)$$

$$P_2(x) = N(m, \sigma^2) \sum_{n=0}^{\infty} (-i\alpha)^n a_n H_n(\alpha(x-m)) \quad (142)$$

Now the characteristic function of the Gaussian is

$$M_1(\theta) = e^{im\theta - \sigma^2\theta^2/2} = e^{im\theta - \theta^2/(4\alpha^2)} \quad (143)$$

giving

$$\Omega(\theta) = \frac{M_2(\theta)}{M_1(\theta)} = M_2(\theta) e^{-im\theta + \theta^2/(4\alpha^2)} \quad (144)$$

in which case

$$a_n = \frac{1}{n!} D^n \frac{M_2(\theta)}{M_1(\theta)} \Big|_{\theta=0} = \frac{1}{n!} D^n M_2(\theta) e^{im\theta - \theta^2/(4\alpha^2)} \Big|_{\theta=0} \quad (145)$$

One can show that

$$a_n = \frac{H_n(\alpha(x-m))}{(-i\alpha)^n 2^n n!} \quad (146)$$

Substituting a_n in Eq. (142) we have

$$P_2(x) = N(m, \sigma^2) \sum_{n=0}^{\infty} \frac{1}{2^n n!} \langle H_n(\alpha(x-m)) \rangle_2 H_n(\alpha(x-m)) \quad (147)$$

If we specialize to the standardized Gaussian ($m = 0, \sigma^2 = 1$) we obtain

$$P_2(x) = N(0, 1) \sum_{n=0}^{\infty} \frac{1}{2^n n!} \langle H_n(x/\sqrt{2}) \rangle_2 H_n(x/\sqrt{2}) \quad (148)$$

Using

$$H_n(x/\sqrt{2}) = 2^{n/2} H e_n(x) \quad (149)$$

results in

$$P_2(x) = N(0, 1) \sum_{n=0}^{\infty} \frac{1}{n!} \langle H e_n(x) \rangle_2 H e_n(x) \quad (150)$$

$$= N(0, 1) \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \langle H e_n(x) \rangle_2 H e_n(x) \right\} \quad (151)$$

which is the standard Gram-Charlier series. This is traditionally derived by different methods [18].

6 Generalization two: the relation between two distributions involving an arbitrary Hermitian operator

We now show that any two densities $P_2(x)$ and $P_1(x)$ can be related by

$$P_2(x) = \Omega(\mathcal{A}) P_1(x) \quad (152)$$

where \mathcal{A} is an arbitrary Hermitian operator, and where now $\Omega(\mathcal{A})$ is given by Eq. (161) below.

For the eigenvalue problem

$$\mathcal{A} u_\theta(x) = \theta u_\theta(x) \quad (153)$$

the eigenfunctions $u_\theta(x)$ form a complete orthogonal set. Hence, any function, and in particular, any probability distribution may be expanded it as

$$P(x) = \int N(\theta) u_\theta(x) d\theta \quad (154)$$

with

$$N(\theta) = \int P(x) u_\theta^*(x) dx \quad (155)$$

Here $N(\theta)$ can be thought of as a generalized characteristic function. The case where $\mathcal{A} = iD$ and $u_\theta(x) = e^{-i\theta x}$ gives the standard characteristic function.

For two probability densities P_1 and P_2 densities with corresponding generalized characteristic functions N_1 and N_2 ,

$$N_1(\theta) = \int P_1(x) u_\theta^*(x) dx \quad N_2(\theta) = \int P_2(x) u_\theta^*(x) dx \quad (156)$$

the distributions are obtained from

$$P_1(x) = \int N_1(\theta) u_\theta(x) d\theta \quad P_2(x) = \int N_2(\theta) u_\theta(x) d\theta \quad (157)$$

Consider $P_2(x)$,

$$P_2(x) = \int N_2(\theta) u_\theta(x) d\theta \quad (158)$$

$$= \int \frac{N_2(\theta)}{N_1(\theta)} N_1(\theta) u_\theta(x) d\theta \quad (159)$$

$$= \int \Omega(\theta) N_1(\theta) u_\theta(x) d\theta \quad (160)$$

where

$$\Omega(\theta) = \frac{N_2(\theta)}{N_1(\theta)} \quad (161)$$

Using

$$\Omega(\theta) u_\theta(x) = \Omega(\mathcal{A}) u_\theta(x) \quad (162)$$

we have

$$P_2(x) = \int u_\theta(x) \Omega(\theta) N_1(\theta) d\theta \quad (163)$$

$$= \Omega(\mathcal{A}) \int N_1(\theta) u_\theta(x) d\theta \quad (164)$$

which gives Eq. (152).

7 Manifestly positive distributions

If one truncates the series previously derived, then generally speaking, the truncated series will not be manifestly positive. We now derive relations between probability densities that even after truncation the series are manifestly positive.

Since Eq. (68), holds for any pair of functions, say F_1 and F_2 , we can write

$$F_2(x) = \Omega(iD)F_1(x) \quad (165)$$

However, here $\Omega(iD)$ is not the ratio of characteristic functions but is given by

$$\Phi(\theta) = \frac{R_2(\theta)}{R_1(\theta)} \quad (166)$$

where

$$R_1(\theta) = \int e^{i\theta x} F_1(x) dx \quad (167)$$

$$R_2(\theta) = \int e^{i\theta x} F_2(x) dx \quad (168)$$

and

$$F_1(x) = \frac{1}{2\pi} \int e^{-i\theta x} R_1(\theta) d\theta \quad (169)$$

$$F_2(x) = \frac{1}{2\pi} \int e^{-i\theta x} R_2(\theta) d\theta \quad (170)$$

We now define F_1 and F_2 by

$$F_1(x) = \sqrt{P_1(x)} e^{i\varphi_1(x)} \quad (171)$$

$$F_2(x) = \sqrt{P_2(x)} e^{i\varphi_2(x)} \quad (172)$$

where $\varphi_1(x)$ and $\varphi_2(x)$ are real functions whose significance will be discussed later. The probability distributions are obtained from the F functions by

$$P_1(x) = |F_1(x)|^2 \quad (173)$$

$$P_2(x) = |F_2(x)|^2 \quad (174)$$

We also have that

$$F_1^2(x) = P_1(x) e^{-2i\varphi_1(x)} \quad (175)$$

$$F_2^2(x) = P_2(x) e^{-2i\varphi_2(x)} \quad (176)$$

From Eq. (165) we have

$$P_2(x) = |F_2(x)|^2 = |\Phi(iD)F_1(x)|^2 \quad (177)$$

or

$$P_2(x) = \left| \Phi(iD) \sqrt{P_1(x)} e^{i\varphi_1(x)} \right|^2 \quad (178)$$

We also have

$$F_2^2(x) = (\Phi(iD)F_1(x))^2 \quad (179)$$

or

$$P_2(x) = e^{-2i\varphi_2(x)} \left(\Phi(iD)\sqrt{P_1(x)}e^{i\varphi_1(x)} \right)^2 \quad (180)$$

which relates the probability distributions and their respective phases.

7.1 Edgeworth type series

We expand $R(\theta)$ as

$$R(\theta) = \exp \left[\sum_{n=1}^{\infty} k_n \frac{i^n}{n!} \theta^n \right] \quad (181)$$

but, we emphasize, that the k_n 's are not cumulants. We thus have that

$$\Phi(\theta) = \frac{R_2(\theta)}{R_1(\theta)} = \exp \left[\sum_{n=1}^{\infty} (k_n^{(2)} - k_n^{(1)}) \frac{i^n}{n!} \theta^n \right] \quad (182)$$

Therefore

$$F_2(x) = \exp \left[\sum_{n=1}^{\infty} (k_n^{(2)} - k_n^{(1)}) \frac{(-1)^n}{n!} D^n \right] F_1(x) \quad (183)$$

and

$$P_2(x) = \left| \exp \left[\sum_{n=1}^{\infty} (k_n^{(2)} - k_n^{(1)}) \frac{(-1)^n}{n!} D^n \right] F_1(x) \right|^2 \quad (184)$$

Now, if the series is truncated

$$P_2(x) \sim \left| \exp \left[\sum_{n=1}^N (k_n^{(2)} - k_n^{(1)}) \frac{(-1)^n}{n!} D^n \right] F_1(x) \right|^2 \quad (185)$$

we still have a manifestly positive approximate distribution. The interpretation of the k_n and the evaluation of Eq. (185) will be discussed in a forthcoming paper.

7.2 Gram-Charlier type series

Similar considerations can be applied to the Gram-Charlier series. The approach is to define

$$R_1(\theta) = \sum_{n=0}^{\infty} a_n^{(1)} u_n^{(1)}(\theta) \quad (186)$$

$$R_2(\theta) = \sum_{n=0}^{\infty} a_n^{(2)} u_n^{(2)}(\theta) \quad (187)$$

and expand

$$\Phi(\theta) = \frac{R_2(\theta)}{R_1(\theta)} = \sum_{n=0}^{\infty} q_n v_n(\theta) \quad (188)$$

and therefore we have

$$P_2(x) = \left| \sum_{n=0}^{\infty} q_n v_n(iD) \sqrt{P_1(x)} e^{i\varphi_1(x)} \right|^2 \quad (189)$$

If the series is truncated

$$P_2(x) \sim \left| \sum_{n=0}^N q_n v_n(iD) \sqrt{P_1(x)} e^{i\varphi_1(x)} \right|^2 \quad (190)$$

we still have a manifestly positive probability density.

7.3 Generalizing to an arbitrary operator

One can generalize the above consideration to an arbitrary operator. Writing

$$F_2(x) = \Omega(\mathcal{A}) F_1(x) \quad (191)$$

Now $\Omega(\mathcal{A})$ is given by

$$\Phi(\theta) = \frac{R_2(\theta)}{R_1(\theta)} \quad (192)$$

where

$$R_1(\theta) = \int u_{\theta}^*(x) F_1(x) dx \quad (193)$$

$$R_2(\theta) = \int u_{\theta}^*(x) F_2(x) dx \quad (194)$$

Also,

$$F_1(x) = \frac{1}{2\pi} \int u_{\theta}(x) R_1(\theta) d\theta \quad (195)$$

$$F_2(x) = \frac{1}{2\pi} \int u_{\theta}(x) R_2(\theta) d\theta \quad (196)$$

As before we define F_1 and F_2 by

$$F_1(x) = \sqrt{P_1(x)} e^{i\varphi_1(x)} \quad (197)$$

$$F_2(x) = \sqrt{P_2(x)} e^{i\varphi_2(x)} \quad (198)$$

The probability distributions are

$$P_1(x) = |F_1(x)|^2 \quad (199)$$

$$P_2(x) = |F_2(x)|^2 \quad (200)$$

and we also have that

$$F_1^2(x) = P_1(x)e^{-2i\varphi_1(x)} \quad (201)$$

$$F_2^2(x) = P_1(x)e^{-2i\varphi_2(x)} \quad (202)$$

We therefore have

$$P_2(x) = |F_2(x)|^2 = |\Phi(\mathcal{A})F_1(x)|^2 \quad (203)$$

or

$$P_2(x) = \left| \Phi(\mathcal{A})\sqrt{P_1(x)}e^{i\varphi_1(x)} \right|^2 \quad (204)$$

We also have

$$F_2^2(x) = (\Phi(\mathcal{A})F_1(x))^2 \quad (205)$$

giving

$$P_2(x) = e^{-2i\varphi_2(x)} \left(\Phi(\mathcal{A})\sqrt{P_1(x)}e^{i\varphi_1(x)} \right)^2 \quad (206)$$

which relates the probability distributions and their respective phases involving an arbitrary operator.

8 Expansion of the probability distribution in orthogonal polynomials

We now present a different approach to approximating probability distributions which is an extension of the standard way that the Gram-Charlier series is obtained [10, 19]. For an orthogonal set of polynomials, $L_n(x)$, with corresponding weighting function, $w(x)$, one has

$$\int w(x)L_n^*(x)L_k(x)dx = N_n\delta_{nk} \quad (207)$$

where N_n are normalization constants. The weighting function is taken to be real. Although the standard polynomials are real we shall assume that they may be complex as that adds to clarity in the sense of Hilbert space notation.

One can define an orthonormal set of functions by

$$u_n(x) = \frac{1}{\sqrt{N_n}} \sqrt{w(x)} L_n(x) \quad (208)$$

in which case,

$$\int u_n^*(x) u_k(x) dx = \delta_{nk} \quad (209)$$

One can expand any function by

$$f(x) = \sum_{n=0}^{\infty} c_n u_n(x) \quad (210)$$

where the coefficients, c_n , are given by

$$c_n = \int f(x) u_n^*(x) dx \quad (211)$$

We now expand, not the probability distribution, but $P(x)/\sqrt{w(x)}$ as

$$\frac{P(x)}{\sqrt{w(x)}} = \sum_{n=0}^{\infty} c_n u_n(x) \quad (212)$$

The c_n 's are then given by

$$c_n = \int \frac{P(x)}{\sqrt{w(x)}} u_n^*(x) dx \quad (213)$$

$$= \int \frac{P(x)}{\sqrt{w(x)}} \frac{1}{\sqrt{N_n}} \sqrt{w(x)} L_n^*(x) dx \quad (214)$$

$$= \frac{1}{\sqrt{N_n}} \int P(x) L_n^*(x) dx \quad (215)$$

and therefore the coefficients are essentially the expectation value of $L_n^*(x)$,

$$c_n = \frac{1}{\sqrt{N_n}} \langle L_n^*(x) \rangle \quad (216)$$

where

$$\langle L_n^*(x) \rangle = \int P(x) L_n^*(x) dx \quad (217)$$

The distribution is then

$$P(x) = \sqrt{w(x)} \sum_{n=0}^{\infty} \frac{1}{\sqrt{N_n}} \langle L_n^*(x) \rangle u_n(x) \quad (218)$$

Substituting $u_n(x)$ as given by Eq. (208) we have

$$P(x) = w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} \langle L_n^*(x) \rangle L_n(x) \quad (219)$$

We now write Eq. (219) for two different distributions

$$P_1(x) = w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} \langle L_n^*(x) \rangle_1 L_n(x) \quad (220)$$

$$P_2(x) = w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} \langle L_n^*(x) \rangle_2 L_n(x) \quad (221)$$

where

$$\langle L_n^*(x) \rangle_1 = \int P_1(x) L_n^*(x) dx \quad (222)$$

$$\langle L_n^*(x) \rangle_2 = \int P_2(x) L_n^*(x) dx \quad (223)$$

Subtracting one distribution from the other in Eqs. (220) and Eq. (221) we have

$$P_2(x) - P_1(x) = w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} [\langle L_n^*(x) \rangle_2 - \langle L_n^*(x) \rangle_1] L_n(x) \quad (224)$$

or

$$P_2(x) = P_1(x) + w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} [\langle L_n^*(x) \rangle_2 - \langle L_n^*(x) \rangle_1] L_n(x) \quad (225)$$

If we assume that

$$L_0^*(x) = 1 \quad (226)$$

then

$$P_2(x) = P_1(x) + w(x) \sum_{n=1}^{\infty} \frac{1}{N_n} (\langle L_n^*(x) \rangle_2 - \langle L_n^*(x) \rangle_1) L_n(x) \quad (227)$$

The $L_n(x)$ are polynomials and hence $\langle L_n(x) \rangle$ can be constructed from the moments.

If we truncate the series

$$P_2(x) = P_1(x) + w(x) \sum_{n=1}^N \frac{1}{N_n} [\langle L_n^*(x) \rangle_2 - \langle L_n^*(x) \rangle_1] L_n(x) \quad (228)$$

then $P_2(x)$ may not be manifestly positive.

8.1 Example: Hermite functions

Using

$$u_n(x; m, \alpha) = \sqrt{\frac{\alpha}{2^n n! \sqrt{\pi}}} H_n(\alpha(x - m)) e^{-\alpha^2(x-m)^2/2} \quad (229)$$

the weighting function is

$$w(x) = e^{-\alpha^2(x-m)^2} \quad (230)$$

and therefore

$$P_2(x) = P_1(x) + e^{-\alpha^2(x-m)^2} \sum_{n=1}^{\infty} \frac{1}{N_n} [\langle H_n(\alpha(x - m)) \rangle_2 - \langle H_n(\alpha(x - m)) \rangle_1] H_n(\alpha(x - m)) \quad (231)$$

with

$$N_n = \sqrt{\pi} 2^n n! / \alpha \quad (232)$$

Explicitly,

$$P_2(x) = P_1(x) + \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2(x-m)^2} \sum_{n=1}^{\infty} \frac{1}{2^n n!} [\langle H_n(\alpha(x - m)) \rangle_2 - \langle H_n(\alpha(x - m)) \rangle_1] H_n(\alpha(x - m)) \quad (233)$$

This is a general expression and is true for any two densities and where α and m are arbitrary.

If we take $P_1(x)$ to be a Gaussian

$$P_1(x) = \sqrt{\frac{1}{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2} \quad (234)$$

we then have

$$\begin{aligned} P_2(x) &= \sqrt{\frac{1}{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2} \\ &+ \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2(x-m)^2} \sum_{n=1}^{\infty} \frac{1}{2^n n!} [\langle H_n(\alpha(x - m)) \rangle_2 - \langle H_n(\alpha(x - m)) \rangle_1] H_n(\alpha(x - m)) \end{aligned} \quad (235)$$

$$(236)$$

Note that α and m are still arbitrary.

If we take

$$m = \mu \quad \alpha = \frac{1}{\sqrt{2}\sigma} \quad (237)$$

then

$$P_2(x) = \sqrt{\frac{1}{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

$$+ \sqrt{\frac{1}{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2} \sum_{n=1}^{\infty} \frac{1}{2^n n!} \left[\left\langle H_n \left(\frac{(x-\mu)}{\sqrt{2}\sigma} \right) \right\rangle_2 - \left\langle H_n \left(\frac{(x-\mu)}{\sqrt{2}\sigma} \right) \right\rangle_1 \right] H_n \left(\frac{(x-\mu)}{\sqrt{2}\sigma} \right) \quad (238)$$

or

$$P_2(x) = \sqrt{\frac{1}{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2} \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{2^n n!} \left[\left\langle H_n \left(\frac{(x-\mu)}{\sqrt{2}\sigma} \right) \right\rangle_2 - \left\langle H_n \left(\frac{(x-\mu)}{\sqrt{2}\sigma} \right) \right\rangle_1 \right] H_n \left(\frac{(x-\mu)}{\sqrt{2}\sigma} \right) \right\} \quad (239)$$

Using

$$H_n(x/\sqrt{2}) = 2^{n/2} He_n(x)$$

gives

$$P_2(x) = \sqrt{\frac{1}{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2} \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\left\langle He_n \left(\frac{(x-\mu)}{\sigma} \right) \right\rangle_2 - \left\langle He_n \left(\frac{(x-\mu)}{\sigma} \right) \right\rangle_1 \right] He_n \left(\frac{(x-\mu)}{\sigma} \right) \right\} \quad (240)$$

For the standardized the Gaussian,

$$\mu = 0 \quad \sigma = 1 \quad (241)$$

Eq. (240) becomes

$$P_2(x) = \sqrt{\frac{1}{2\pi}} e^{-x^2/2} \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{n!} [\langle He_n(x) \rangle_2 - \langle He_n(x) \rangle_1] He_n(x) \right\} \quad (242)$$

Since

$$\langle He_n(x) \rangle_1 = 0$$

we have

$$P_2(x) = \sqrt{\frac{1}{2\pi}} e^{-x^2/2} \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \langle He_n(x) \rangle_2 He_n(x) \right\} \quad (243)$$

which is the same as Eq. (151) and which is the standard Gram-Charlier series [18] but derived in a different way.

Now if we take $P_2(x)$ to be standardized, then

$$\langle He_1(x) \rangle_2 = 0 \quad (244)$$

$$\langle He_2(x) \rangle_2 = 0 \quad (245)$$

$$\langle He_3(x) \rangle_2 = \langle x^3 \rangle_2 \quad (246)$$

$$\langle He_4(x) \rangle_2 = \langle x^4 \rangle_2 - 6 + 3 = \langle x^4 \rangle_2 - 3 \quad (247)$$

$$\langle He_5(x) \rangle_2 = \langle x^5 \rangle_2 - 10 \langle x^3 \rangle_2 \quad (248)$$

$$\langle He_6(x) \rangle_2 = \langle x^6 \rangle_2 - 15 \langle x^4 \rangle_2 + 45 - 15 = \langle x^6 \rangle_2 - 15 \langle x^4 \rangle_2 + 30 \quad (249)$$

then

$$P_2(x) \sim \sqrt{\frac{1}{2\pi}} e^{-x^2/2} \left\{ 1 + \frac{1}{6} \langle x^3 \rangle_2 He_3(x) + \frac{\langle x^4 \rangle_2 - 3}{24} He_4(x) \right. \\ \left. + \frac{\langle x^5 \rangle_2 - 10 \langle x^3 \rangle_2}{120} He_5(x) + \frac{\langle x^6 \rangle_2 - 15 \langle x^4 \rangle_2 + 30}{720} He_6(x) \dots \right\} \quad (250)$$

Using the relation between moments and cumulants

$$\langle x^3 \rangle_2 = \kappa_3^{(2)} \quad (251)$$

$$\langle x^4 \rangle_2 = \kappa_4^{(2)} + 3 \quad (252)$$

$$\langle x^5 \rangle_2 = \kappa_5^{(2)} + 10 \kappa_3^{(2)} \quad (253)$$

$$\langle x^6 \rangle_2 = \kappa_6^{(2)} + 15 \kappa_4^{(2)} + 10 \left(\kappa_3^{(2)} \right)^2 + 15 \quad (254)$$

one obtains

$$P_2(x) \sim \left\{ 1 + \frac{1}{6} \kappa_3^{(2)} He_3(x) + \frac{1}{24} \kappa_4^{(2)} He_4(x) + \frac{1}{120} \kappa_5^{(2)} He_5(x) \right. \\ \left. + \frac{1}{720} \left(\kappa_6^{(2)} + 10 \left(\kappa_3^{(2)} \right)^2 \right) He_6(x) + \dots \right\} N(0, 1) \quad (255)$$

which is the same as Eq. (131).

8.2 Example: Laguerre polynomials

The Laguerre polynomials are defined by

$$L_n(x) = \sum_{k=0}^n \frac{(-1)^{n-k} n! x^{n-k}}{k! [(n-k)!]^2} = \frac{e^x}{n!} \frac{d^k}{dx^k} x^n e^{-x} \quad (256)$$

The weighting function for the Laguerre polynomials is

$$w(x) = e^{-x} \quad (257)$$

and the normalization is

$$\int_0^\infty e^{-x} L_n(x) L_k(x) dx = \delta_{nk} \quad (258)$$

Therefore for the Laguerre polynomials

$$N_n = 1 \quad (259)$$

We use the following orthonormal set

$$u_n(x; \beta) = \sqrt{\beta} \sqrt{w(\beta x)} L_n(\beta x) = \sqrt{\beta} e^{-\beta x/2} L_n(\beta x) \quad (260)$$

where β is a positive number. From Eq. (258) we have

$$\int u_n(x; \beta) u_k(x; \beta) dx = \delta_{nk} \quad (261)$$

with weighting function

$$w(x) = \beta e^{-\beta x} \quad (262)$$

Using Eq. (227) we may write

$$P_2(x) = P_1(x) + \beta e^{-\beta x} \sum_{n=1}^{\infty} [\langle L_n(\beta x) \rangle_2 - \langle L_n(\beta x) \rangle_1] L_n(\beta x) \quad (263)$$

This is general. If we take the exponential probability distribution for $P_1(x)$

$$P_1(x) = \beta e^{-\beta x} \quad (264)$$

then

$$P_2(x) = \beta e^{-\beta x} \left\{ 1 + \sum_{n=1}^{\infty} [\langle L_n(\beta x) \rangle_2 - \langle L_n(\beta x) \rangle_1] L_n(\beta x) \right\} \quad (265)$$

which allows one to correct the exponential distribution, Eq. (131).

8.3 Legendre Polynomials

The Legendre polynomials allow one to correct distributions which are uniform in an interval. The Legendre polynomials are

$$P_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k (2n-2k)!}{2^n k! (n-k)! (n-2k)!} x^{n-2k} = \frac{1}{2^n n!} \left(\frac{d}{dx} \right)^n (x^2 - 1)^n \quad (266)$$

and the orthogonality condition is

$$\int_{-1}^1 P_n(x) P_k(x) dx = \frac{2}{2n+1} \delta_{nk} \quad (267)$$

The normalization constant are therefore

$$N_n = \frac{2}{2n+1} \quad (268)$$

We define the complete set of functions by

$$u_n(x; \beta) = \sqrt{\frac{2n+1}{2}} \frac{1}{\sqrt{\beta}} P_n(x/\beta) \quad (269)$$

so that the $u_n(x; \beta)$ are orthonormal in the interval $-\beta$ to β

$$\int_{-\beta}^{\beta} u_n(x; \beta) u_k(x; \beta) dx = \delta_{nk} \quad (270)$$

Using Eq. (227) we have

$$f_2(x) = f_1(x) + \frac{1}{\beta} \sum_{n=1}^{\infty} \frac{1}{N_n} [\langle P_n(x/\beta) \rangle_2 - \langle P_n(x/\beta) \rangle_1] P_n(x/\beta) \quad -\beta \leq x \leq \beta \quad (271)$$

where we have used $f(x)$ for the probability density to avoid confusion with the Legendre polynomials.

If we take the uniform probability distribution for $f_1(x)$

$$f_1(x) = \frac{1}{2\beta} \quad -\beta \leq x \leq \beta \quad (272)$$

then

$$f_2(x) = \frac{1}{2\beta} + \frac{1}{\beta} \sum_{n=1}^{\infty} \frac{1}{N_n} [\langle P_n(x/\beta) \rangle_2 - \langle P_n(x/\beta) \rangle_1] P_n(x/\beta) \quad -\beta \leq x \leq \beta \quad (273)$$

or

$$f_2(x) = \frac{1}{2\beta} \left\{ 1 + 2 \sum_{n=1}^{\infty} \frac{1}{N_n} [\langle P_n(x/\beta) \rangle_2 - \langle P_n(x/\beta) \rangle_1] P_n(x/\beta) \right\} \quad -\beta \leq x \leq \beta \quad (274)$$

8.4 Obtaining manifestly positive distributions by expanding the state function

Eq. (227) holds for any two functions $F_2(x)$ and $F_1(x)$, not just probability distributions. Hence we may write

$$F_2(x) = F_1(x) + w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} [\langle L_n^*(x) \rangle_2 - \langle L_n^*(x) \rangle_1] L_n(x) \quad (275)$$

where now

$$\langle L_n^*(x) \rangle_1 = \int F_1(x) L_n^*(x) dx \quad (276)$$

$$\langle L_n^*(x) \rangle_2 = \int F_2(x) L_n^*(x) dx \quad (277)$$

and we note that $\langle L_n^*(x) \rangle$ are not expectation values since the F 's are not probability density functions.

As before, we define

$$F_1(x) = \sqrt{P_1(x)} e^{i\varphi_1(x)} \quad (278)$$

$$F_2(x) = \sqrt{P_2(x)} e^{i\varphi_2(x)} \quad (279)$$

Therefore

$$P_2(x) = \left| \sqrt{P_1(x)} e^{i\varphi_1(x)} + w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} (\langle L_n^*(x) \rangle_2 - \langle L_n^*(x) \rangle_1) L_n(x) \right|^2 \quad (280)$$

and

$$P_2(x) = e^{-2i\varphi_2(x)} \left(\sqrt{P_1(x)} e^{i\varphi_1(x)} + w(x) \sum_{n=0}^{\infty} \frac{1}{N_n} (\langle L_n^*(x) \rangle_2 - \langle L_n^*(x) \rangle_1) L_n(x) \right)^2 \quad (281)$$

If we truncate the series we still have a manifestly positive expression.

9 Conclusion

We have generalized the Edgeworth and Gram-Charlier types of series in a number of ways, and have also shown how to modify these series so that even after truncation the series remain manifestly positive. What we have not shown is the physical meaning of the phases

as defined in Eq. (171) and Eq. (172). We believe that we can relate these phases to the moments and cumulants and other expectation values and this is currently being investigated along the lines of Davidson and Loughlin [11, 12, 14].

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